

# High quality quant

Examples of high quality quant

Thanks to Dale Newbury for many of the examples

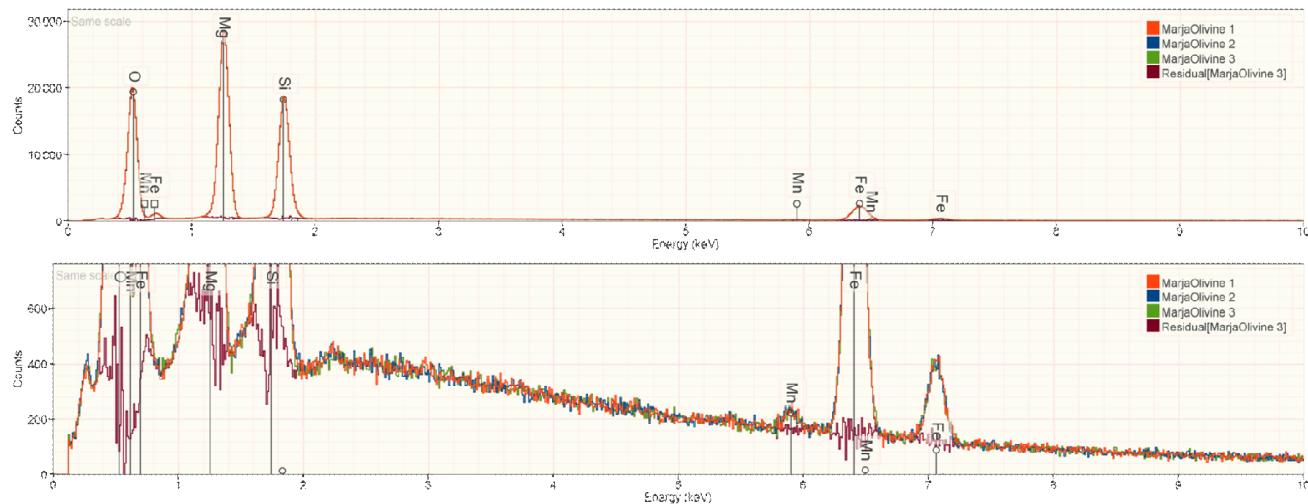
# Types of challenges

- Simple Trace
  - 0.2 % Mn in an Olivine
- Interferences
  - 1.7 % Ti in Ba-Ti glasses
- Trace interferences
  - 0.4% Ce and 0.4 % Ta in K873 glass
- Light elements
  - Carbides, Nitrides and Oxides... Oh my!



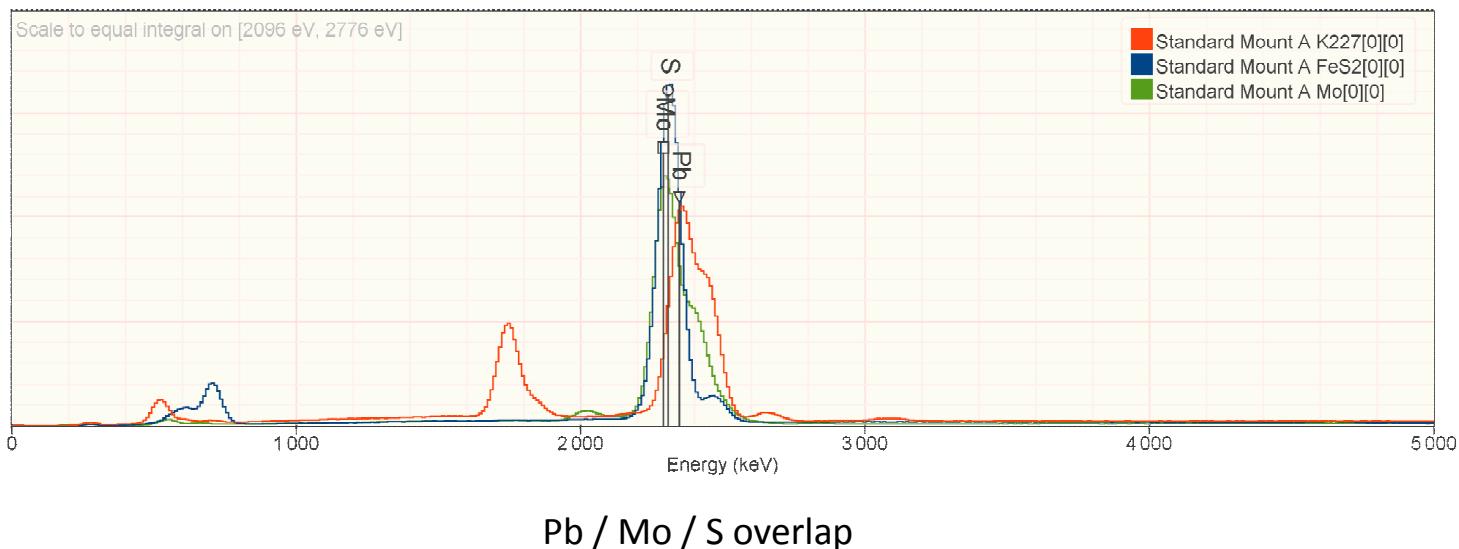
# Marja Olivine

Name	O	Mg	Si	Mn	Fe
MarjaOlivine 1	42.78	28.44	18.79	0.23	8.99
MarjaOlivine 2	42.58	28.34	18.70	0.22	8.91
MarjaOlivine 3	42.82	28.62	18.76	0.21	8.85
Average	42.72	28.47	18.75	0.22	8.92
Std. Dev.	0.10	0.11	0.03	0.01	0.05
Nominal	43.3	29.0	18.8	0.2	8.7

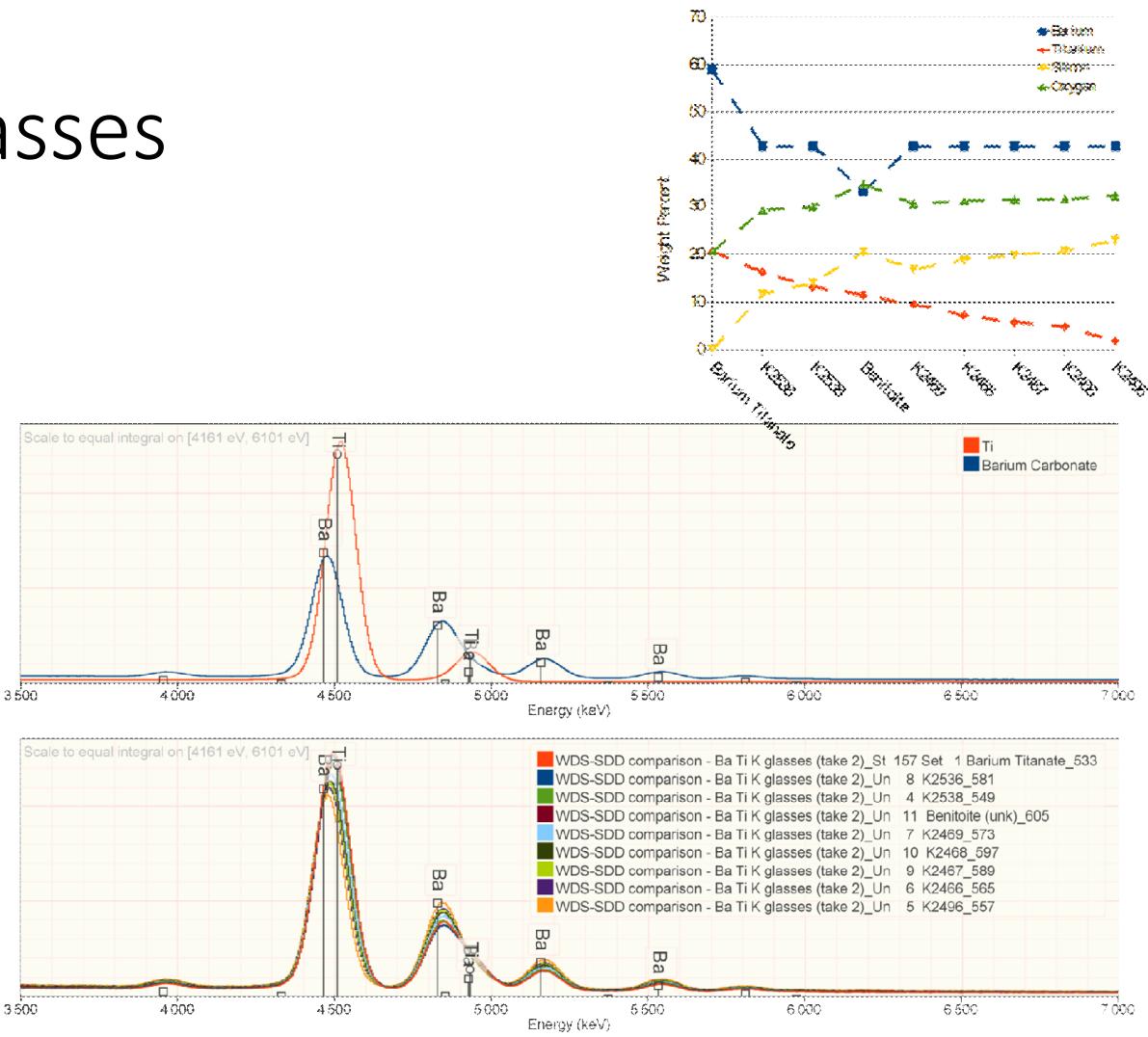


# Interferences

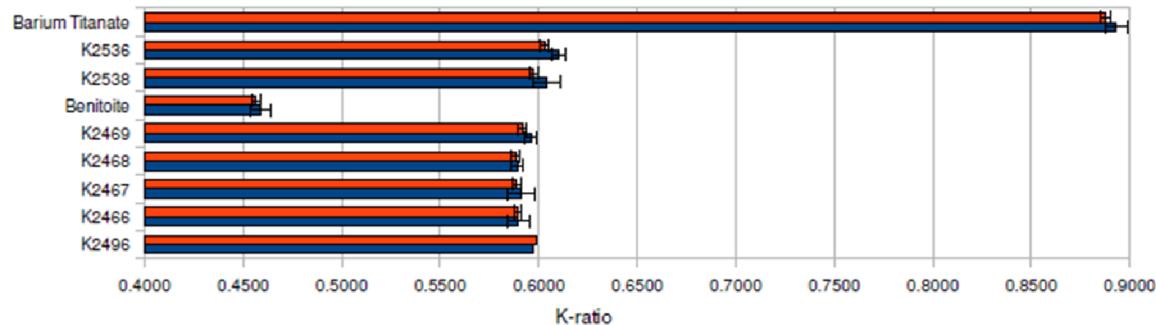
Photon energy range (keV)	Element (energy)
0.390-0.395	N K (0.392); ScL (0.395)
0.510-0.525	O K (0.523); V L (0.511)
0.670-0.710	F K (0.677); FeL (0.705)
0.845-0.855	NeK (0.848); NiL (0.851)
1.00-1.05	NaK (1.041); ZnL (1.012); PmM (1.032)
1.20-1.30	MgK (1.253); AsL (1.282); TbM (1.246)
1.45-1.55	AlK (1.487); BrL (1.480); YbM (1.521)
1.70-1.80	SiK (1.740); RbL (1.694); SrL (1.806); TaM (1.709); W M (1.774)
1.90-1.99	Y L (1.922); OsM (1.910)
2.00-2.05	PK (2.013); ZrL (2.042); PtM (2.048)
2.10-2.20	NbL (2.166); AuM (2.120); HgM (2.191)
2.28-2.35	S K (2.307); MoL (2.293); PbM (2.342)
2.40-2.45	TcL (2.424); BiM (2.419)
2.60-2.70	CfK (2.621); RhL (2.696)
2.95-3.00	ArK (2.956); AgL (2.983); ThM (2.996)
3.10-3.20	CdL (3.132); U Ma (3.170)
3.25-3.35	K Ka (3.312); InLa (3.285); U Mb (3.336)
4.45-4.55	TiKa (4.510); BaLa (4.467)



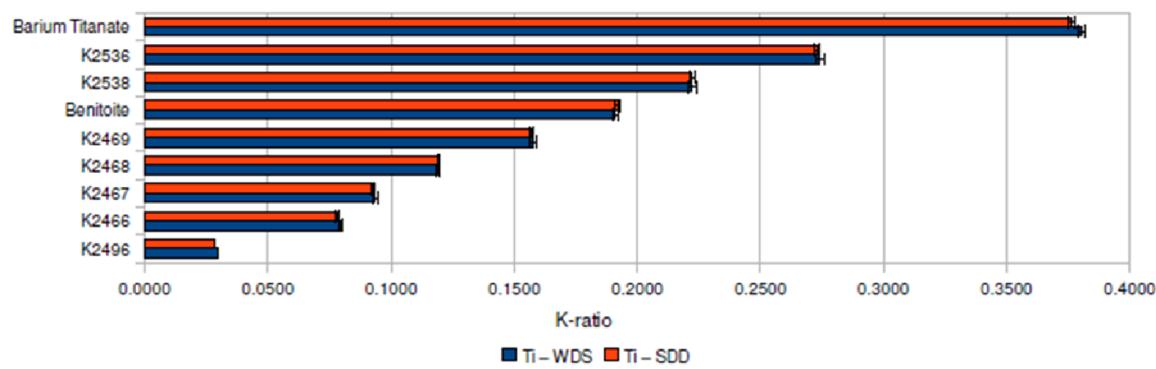
# Ba-Ti glasses



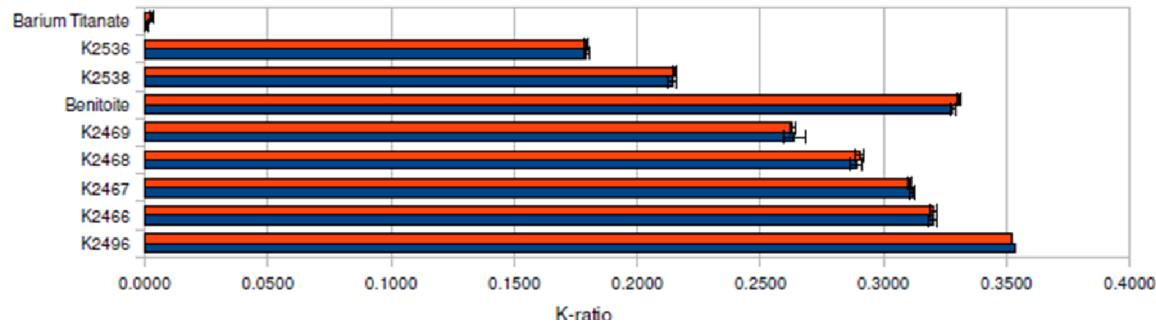
### Barium La



### Titanium Ka



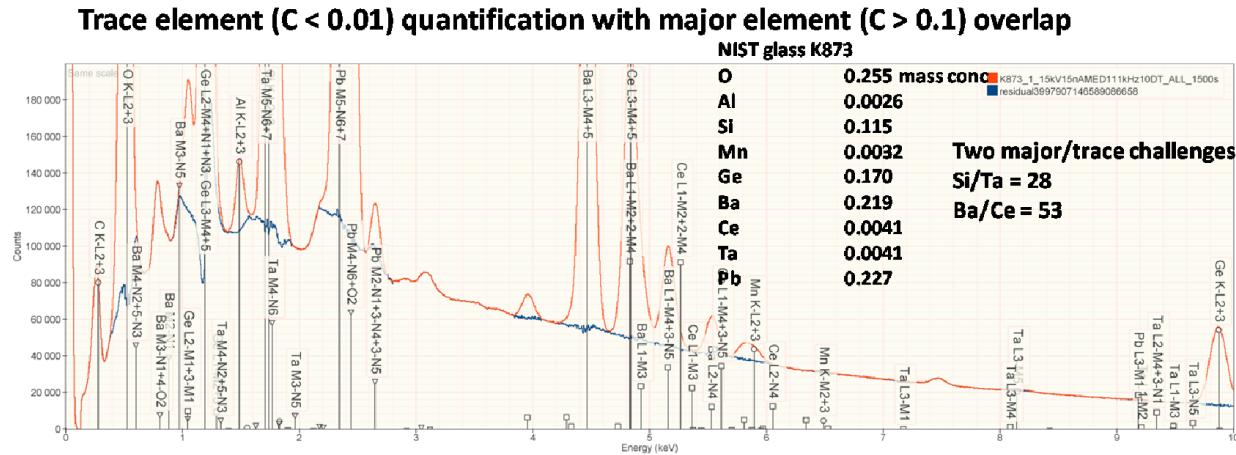
### Silicon Ka



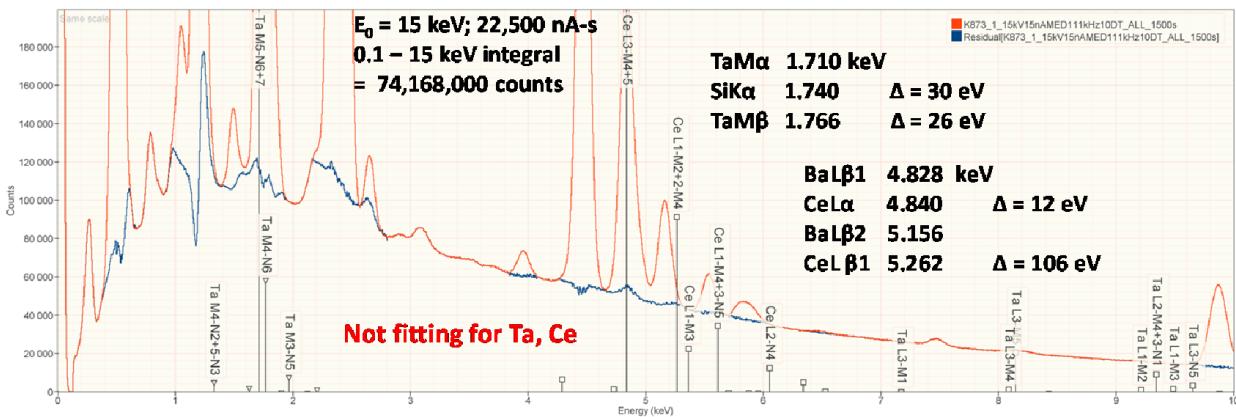
# K2496 glass

Parameter	O, mass conc	Si, mass conc	Ti, mass conc	Ba, mass conc
Concentration (as-synthesized)	0.3230	0.2291	0.0180	0.4299
Concentration (average of 7 locations)	0.3197	0.2256	0.0176	0.4371
Relative error, %	-1.0%	-1.5%	-2.4%	1.7%
$\sigma$	0.00024	0.00028	0.00031	0.00058
$\sigma$ relative, %	0.08%	0.13%	1.8%	0.13%
Error in k	NA	0.0001	0.0003	0.0007
Rel err, %		0.044%	1.7%	0.16%
Error in Z	NA	0.000011	0.00000025	0.00000021
Rel err, %		0.0049%	0.0014%	0.000048%
Error in A	NA	0.0015	0.0000039	0.000019
Rel err, %		0.66%	0.022%	0.0043%
Combined errors	NA	0.0015 0.66%	0.0003 1.7%	0.0007 0.16%

# Trace interference - K873 glass



**Could we find the trace Ce and Ta if we did not know in advance they were present?**



# Trace interference - K873 glass

Ba L on Ce L (54/1) and Si K on Ta M (28/1)

Parameter	O stoi	Al	Si	Mn	Ge	Ba	Ce	Ta	Pb
Concentration synthesized	0.2547	0.00265	0.1145	0.00316	0.1700	0.2194	0.00407	0.0041	0.2274
Concentration (average of 8 locations)	0.2556	0.00310	0.1151	0.00279	0.1728	0.2205	0.00489	0.00329	0.2282
Relative error, %	0.37%	17%	0.49%	-12%	1.6%	0.50%	20%	-20%	0.34%
$\sigma$	0.0004	0.000033	0.00013	0.00015	0.00045	0.00013	0.00039	0.00009	0.00033
$\sigma$ relative, %	0.15%	1.1%	0.11%	5.4%	0.26%	0.06%	8.0%	2.7%	0.14%
Error in k	NA	3.3E-5	0.0001	0.0004	0.0001	0.0007	0.0008	0.0003	0.0004
Rel err, %		1.1%	0.085%	14%	0.06%	0.32%	16%	1.6%	0.18%
Error in Z	NA	1.5E-9	1.8E-6	3.1E-11	1E-5	4.8E-7	2.1E-10	3.2E-9	6.5E-6
Rel err, %		0.0%	0.0015%	0.0%	0.006%	0.00%	0.00%	0.00%	0.00%
Error in A	NA	3.5E-7	7.5E-5	3.4E-8	0.0015	0.0002	5.4E-8	4.5E-7	0.0004
Rel err, %		0.011%	0.064%	0.0%	0.87%	0.00%	0.00%	0.00%	0.18%
Combined errors	NA	3.3E-5	0.0001	0.0004	0.0015	0.00072	0.0008	0.0003	0.00057
		1.1%	0.085%	14%	0.87%	0.33%	16%	1.6%	0.25%

# Carbides, Nitrides and Oxides

SEM/SDD-EDS analysis of metal carbides (results in atom fractions)

Carbide	C ideal	C mean	Relative error, %	$\sigma$	Relative $\sigma$ , %	metal ideal	metal mean	Relative error, %	$\sigma$	Relative $\sigma$ , %
$\text{Cr}_3\text{C}_2$	0.4000	0.3967	-0.83%	0.0029	0.73%	0.6000	0.6033	0.55%	0.0029	0.48%
$\text{Cr}_7\text{C}_3$	0.3000	0.2961	-1.3%	0.0098	3.3%	0.7000	0.7039	0.57%	0.0098	1.4%
$\text{Cr}_{23}\text{C}_6$	0.2069	0.2069	0%	0.0039	1.9%	0.7931	0.7931	0%	0.0039	0.49%
$\text{Fe}_3\text{C}$	0.2500	0.2469	-1.2%	0.00085	0.35%	0.7500	0.7531	0.42%	0.00085	0.11%

SEM/SDD-EDS analysis of metal nitrides (results in atom fractions)

Nitride	N ideal	N mean	Relative error, %	$\sigma$	Relative $\sigma$ , %	metal ideal	metal mean	Relative error, %	$\sigma$	Relative $\sigma$ , %
TiN	0.5000	0.5098	2.0%	0.00156	0.3%	0.5000	0.4902	-2.0%	0.00156	0.32%
VN	0.3000	0.2961	-1.3%	0.0098	3.3%	0.7000	0.7039	0.57%	0.0098	1.4%
$\text{Cr}_2\text{N}$	0.3333	0.3501	5.1%	0.006	1.7%	0.6667	0.6499	-2.5%	0.006	0.93%
$\text{Fe}_3\text{N}$	0.2500	0.2573	2.9%	0.00688	2.7%	0.7500	0.7427	-1.0%	0.00688	0.90%

SEM/SDD-EDS analysis of metal oxides (results in atom fractions)

Oxide	O ideal	O mean	Relative error, %	$\sigma$	Relative $\sigma$ , %	metal ideal	metal mean	Relative error, %	$\sigma$	Relative $\sigma$ , %
$\text{Al}_2\text{O}_3$	0.6000	0.5905	-1.6%	0.00039	0.07%	0.4000	0.4095	2.4%	0.00039	0.1%
$\text{SiO}_2$	0.6667	0.6535	-2.0%	0.00033	0.05%	0.3333	0.3465	4.0%	0.00033	0.1%
SiO	0.5000	0.4989	-0.20%	0.00033	0.07%	0.5000	0.5011	0.20%	0.00033	0.07%
$\text{Fe}_2\text{O}_3$	0.6000	0.5988	-0.20%	0.00068	0.11%	0.4000	0.4012	0.30%	0.00068	0.17%
$\text{Cu}_2\text{O}$	0.3333	0.3250	-2.5%	0.0010	0.30%	0.6667	0.6750	1.2%	0.0010	0.15%
CuO	0.5000	0.4868	-2.6%	0.0026	0.54%	0.5000	0.5132	2.6%	0.0026	0.51%

# And there is more...

SEM/SDD-EDS Analysis of Sulfides with NIST DTSA II k-ratio protocol with various standards, including pure elements and other sulfides ( $E_0 = 20$  keV)

Compound	Metal	Analysis	Relative Error (%)	Sulfur	Analysis	Relative Error (%)
FeS	0.635	0.635	0	0.365	0.365	0
FeS <sub>2</sub>	0.466	0.463	-0.6	0.534	0.537	0.6
CuS	0.665	0.667	0.3	0.335	0.333	-0.6
ZnS	0.671	0.674	0.4	0.329	0.326	-0.9
SrS	0.732	0.737	0.7	0.268	0.263	-1.9
CdS	0.778	0.786	1	0.222	0.214	-3.6
Sb <sub>2</sub> S <sub>3</sub>	0.717	0.727	1.4	0.283	0.273	-3.5
PbS	0.866	0.87	0.5	0.134	0.13	-3